On exotic sphere fibrations, topological phases, and edge states in physical systems

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Abstract

We suggest that exotic sphere fibrations can be mapped to band topologies in condensed matter systems. These fibrations can correspond to geometric phases of two double bands or state vector bases with second Chern numbers $m + n$ and $-n$ respectively. They can be related to topological insulators, magneto-electric effects, and photonic crystals with special edge states. We also consider time-reversal symmetry breaking perturbations of topological insulator, and heterostructures of topological insulators with normal insulators and with superconductors. We consider periodic TI/NI/TI/NI′ heterostuctures, and periodic TI/SC/TI/SC′ heterostuctures. They also give rise to models of Weyl semimetals which have thermal and electrical transports.

I. INTRODUCTION

In this article, we propose to realize the exotic spheres as the geometric phases in condensed matter systems. We suggest that the exotic sphere fibration can be realized as the geometric phases in condensed matter systems, cold atomic or molecular systems.

The topological description of the quantum states of matter gives a new method in describing the condensed matter. Condensed matter systems with band structures that have nontrivial topological properties give a new type of materials with properties that are robust under certain perturbations. There are many interesting topological properties for example the appearance of edge states and the existence of gapless surface states.

The topological insulator has a bulk gap, while it has topologically protected edge states on the boundary of the topological insulator. Thus, the topological insulator is an insulator in the bulk while has gapless edge states on the boundary of the topological insulator. The 3D topological insulators have been shown in materials for example,[1–4] Bi_2Te_3, Bi_2Se_3, Sb_2Te_3, $Bi_{1-x}Sb_x$. The 2D topological insulators have been observed in HgTe quantum wells.[5,6]

For the 3D topological insulators, the topologically protected surface state realizes itself by the non-trivial spin texture on the surface band of the topological insulator. The topological surface state is protected by time-reversal symmetry. The existence of odd number of or single surface Dirac point is robust in the presence of nonmagnetic impurities, and other time-reversal symmetry preserving perturbations. The difference between topological insulator and normal insulator can be distinguished by a Z_2 invariant.[7–9] The 3D topological insulators can be described[10] by topological field theory with a θ variable. Due to the time reversal symmetry, θ takes values of 0 or π, modulo 2π. The θ term gives magnetoelectric effects, with magnetoelectric polarization in the materials.[10,11] The spin polarization of surface band and magnetoelectric polarization of the materials, can be experimentally measured.

In early days of differential topology, John Milnor constructed a seven dimensional compact space called exotic sphere. The space he constructed has the property that it has a continuous one to one map to the round sphere, and yet it cannot be mapped to the round sphere smoothly. There are 28 Milnor exotic spheres that are mutually distinct from each other. The construction was based on distinct bundles over the four dimensional manifold. Bundles over four dimensional manifold may be used to describe geometric phases in con-

densed matter and atomic systems. It is interesting to see whether one can build the Milnor exotic spheres into the theory of condensed matter and atomic systems. It is also nice to connect subjects in mathematics to subjects in theoretical physics.

In this paper, we suggest that exotic sphere fibrations can be mapped to band topologies in condensed matter systems. These fibrations can be mapped to geometric phases of two double bands or state vector bases with their associated second Chern numbers. They can be related to topological insulators, magneto-electric effects, and photonic crystals with special edge states, among other aspects. It is nice to understand the physics of topological insulator in the situations when it is placed adjacent to other kinds of materials. We also consider time-reversal symmetry breaking perturbations of topological insulator, and heterostructures of topological insulators with normal insulators and with superconductors.

The organization of this article is as follows. In section II, we discuss that exotic sphere fibrations can be related to band topologies in condensed matter systems. These fibrations can be mapped to geometric phases of two double bands or state vector bases with the second Chern numbers $m+n$ and $-n$ respectively. In section III, we discuss their relation to topological insulators, and magneto-electric effects. In section IV, we also discuss their relation to photonic crystals with special edge states. In section V, we consider time-reversal symmetry breaking perturbations of topological insulator, and heterostructures of topological insulators with normal insulators, and periodic TI/NI/TI/NI′ heterostuctures. In section VI, we consider heterostructures of topological insulators with superconductors, and periodic TI/SC/TI/SC′ heterostuctures. These structures also give rise to models of Weyl semimetals which have thermal and electrical transports. In section VII, we also suggest relevance to other possible materials such as cold atom systems and semiconductor systems.

II. GEOMETRIC PHASES OF TWO DOUBLE BANDS OR STATE VECTOR BASES AND RELATED TOPOLOGIES

One of the interesting types of fiber bundles are 3-sphere bundles over 4-sphere. Such fibrations can be constructed by patching two $R^4 \times S^3$ and identify their overlapping region by a diffeomorphism. One can divide S^4 into three regions: a north patch $R^4_{(1)}$; a middle patch $[-\epsilon, \epsilon] \times S^3$; and a south patch $R^4_{(2)}$. The $R^4_{(1)} \times S^3$ can be parametrized by a quaternion

u and a unit norm quaternion v, in which the u belongs to the $R^4_{(1)}$ and the v belongs to the S^3. Similarly, the $R^4_{(2)} \times S^3$ can be parametrized by a quaternion u' and a unit norm quaternion v'. The transition function is defined on the middle patch, and it is

$$u' = \frac{u}{\|u\|^2}, \qquad v' = \frac{u^m(u^n v u^{-n})}{\|u\|^m} = \frac{u^{n+m}(v)u^{-n}}{\|u\|^m}. \tag{1}$$

$\|u\|$ denotes the norm of the quaternion u, while $\|v'\| = \|v\| = 1$. Such fibrations can be classified by two integers $(n+m, -n)$.

The fibration of S^3 over S^4 can be characterized by the map from the middle patch S^3 to the structure group $SO(4)$ which corresponds to the rotational symmetry of the S^3 fiber. This map is characterized by homotopy group $\pi_3(SO(4)) \cong \mathrm{Z} \oplus \mathrm{Z},$ where $\pi_3(SU(2)) \cong \mathrm{Z},$ and $so(4) = su(2)_{(1)} \times su(2)_{(2)}$. This fibration is characterized by two integers, which correspond to $(n+m, -n)$. The two integers $n+m$ and $-n$ correspond to the second Chern numbers of the $su(2)_{(1)}$ and $su(2)_{(2)}$. This may be viewed as

$$c_2^{(1)} = \frac{1}{8\pi^2}\int (\mathrm{tr}F^{(1)} \wedge F^{(1)}) = n+m, \tag{2}$$

$$c_2^{(2)} = \frac{1}{8\pi^2}\int (\mathrm{tr}F^{(2)} \wedge F^{(2)}) = -n, \tag{3}$$

and the integration is on the four dimensional base manifold.

This can be interpreted as $n+m$ instantons of the $su(2)_{(1)}$ gauge fields, and n anti-instantons of the $su(2)_{(2)}$ gauge fields. This can also be viewed as m instantons of $su(2)_{(1)}$, plus n pairs of $su(2)_{(1)}$ instanton and $su(2)_{(2)}$ anti-instanton. For $m = 1$, different n are in different diffeomorphism classes, but in the same homeomorphism class. The standard sphere corresponds to $n = 0$, $m = 1$, which also corresponds to one instanton of $su(2)_{(1)}$ on S^4. For $n > 0$, $m = 1$, it is the exotic sphere, and it also corresponds to $n+1$ instantons of $su(2)_{(1)}$, and n anti-instantons of $su(2)_{(2)}$. The case for $m = 2$, and other general m, are also very interesting.

We propose to realize exotic sphere fibrations (2, 3) by geometric phases in condensed matter systems, cold atomic systems or molecular systems. These exotic fibrations can be mapped to band structures of those systems with nontrivial band topologies in the systems.

We start with wavefunction $\left|\psi^I\right\rangle$, where I labels bands in band structure, or labels state vector bases, and define gauge field associated with the geometric phase in parameter space,

$$A_a^{(1)ij} = -i\left\langle\psi^i(\{\xi_a\})\right|\partial_{\xi_a}\left|\psi^j(\{\xi_a\})\right\rangle, \tag{4}$$

$$A_a^{(2)\alpha\beta} = -i \langle \psi^\alpha(\{\xi_a\}) | \, \partial_{\xi_a} \left| \psi^\beta(\{\xi_a\}) \right\rangle , \tag{5}$$

where i, j, α, β label different bands, or state vector bases. ξ_a are parameters for the wavefunctions. The i, j labels a double band and takes values 1 or 2. The α, β labels a different double band and takes values 1 or 2. We have written the states in orthonormal basis. When the two bands are degenerate or almost degenerate, the geometric phase becomes a non-abelian matrix-valued quantity. ξ_a are the coordinates on the parameter space. $(\xi_1, \xi_2, \xi_3, \xi_4)$ parametrize four dimensional manifold. Since there are two $su(2)$ gauge fields, the band structure is such that there are four occupied bands, and there are two $su(2)$ gauge fields associated with the two double bands in the parameter space. The two bands in the double band will be degenerate at some points of the parameter space, the ξ space.

The four-parameter space can be momentum space, or it can be momentum space together with extra parameters, or it can be other parameters in the model. It is good to embed a three dimensional experimental system into a four dimensional parameter space. For example, the four dimensional parameter space $(\xi_1, \xi_2, \xi_3, \xi_4)$ can be three dimensional momentum space (k_1, k_2, k_3) with an additional parameter ξ_4. ξ_4 can be a parameter in the model Hamiltonian or the effective model of the experimental system. ξ_4 can also be k_4, or ω, or a parameter in the model Hamiltonian. It can also be two dimensional momentum space (k_1, k_2) with additional parameters ξ_4, ξ_3. It can also be real space, together with additional parameters.

The geometric phase is sometimes also called the holonomy. Under the adiabatic evolution along a closed path in the parameter space, the state vector will come back to itself up to an extra unitary phase factor, given by the integration of path ordered exponential of the Berry holonomy along that path.

We look for experimental quantities that can be realized from the structures of (2, 3). The field strengthes are

$$F_{ab}^{(1)ij} = -i \left\langle \partial_a \psi^i \, \middle| \partial_b \psi^j \right\rangle + i \left\langle \partial_b \psi^i \, \middle| \partial_a \psi^j \right\rangle + i \left\langle \psi^i \, \middle| \partial_a \psi^l \right\rangle \left\langle \psi^l \, \middle| \partial_b \psi^j \right\rangle - i \left\langle \psi^i \, \middle| \partial_b \psi^l \right\rangle \left\langle \psi^l \, \middle| \partial_a \psi^j \right\rangle , \tag{6}$$

$$F_{ab}^{(2)\hat{\imath}\hat{\jmath}} = -i \left\langle \partial_a \psi^{\hat{\imath}} \, \middle| \partial_b \psi^{\hat{\jmath}} \right\rangle + i \left\langle \partial_b \psi^{\hat{\imath}} \, \middle| \partial_a \psi^{\hat{\jmath}} \right\rangle + i \left\langle \psi^{\hat{\imath}} \, \middle| \partial_a \psi^{\hat{l}} \right\rangle \left\langle \psi^{\hat{l}} \, \middle| \partial_b \psi^{\hat{\jmath}} \right\rangle - i \left\langle \psi^{\hat{\imath}} \, \middle| \partial_b \psi^{\hat{l}} \right\rangle \left\langle \psi^{\hat{l}} \, \middle| \partial_a \psi^{\hat{\jmath}} \right\rangle , \tag{7}$$

a, b label the parameter space, and i, j label the state vector bases or bands. The bracket denotes the inner product of wavefunctions in the Hilbert space. One interesting situation

is when $\xi_a = k_a$, $a = 1, 2, 3$, and ξ_4 is an additional parameter, and this correspond to the momentum space of 3D materials. Summation of the scripts are assumed in the notations.

Moreover, there are second Chern numbers $c_2^{(1)}, c_2^{(2)}$ of these two gauge fields,

$$c_2^{(1)} = \frac{1}{8\pi^2} \int (\mathrm{tr} F^{(1)} \wedge F^{(1)}) = \frac{1}{32\pi^2} \int d^4\xi \ \epsilon_{abcd} (\mathrm{tr} F^{(1)}_{ab} F^{(1)}_{cd}), \tag{8}$$

$$c_2^{(2)} = \frac{1}{8\pi^2} \int (\mathrm{tr} F^{(2)} \wedge F^{(2)}) = \frac{1}{32\pi^2} \int d^4\xi \ \epsilon_{abcd} (\mathrm{tr} F^{(2)}_{ab} F^{(2)}_{cd}), \tag{9}$$

where the integration is on the parameter space $(\xi_1, \xi_2, \xi_3, \xi_4)$ and $d^4\xi = d\xi_1 d\xi_2 d\xi_3 d\xi_4$. The second Chern numbers are

$$c_2^{(1)} = n + m, \quad c_2^{(2)} = -n. \tag{10}$$

The non-trivial Chern numbers correspond to the non-trivial topology of the band structure. It is an S^3 fibration of four-sphere. The $su(2)$ fibration on the 4d parameter space realizes a higher dimensional manifold. The (8, 9) can also be interpreted as four-form magnetic monopole fluxes on the parameter space.

Realization and interpretation of the two $su(2)$'s and the parameter space can be diverse, in condensed matter and atomic systems. This type of fibration are still abstract. It can be mapped to band structures in different possible systems. It has relevance to both electron band structures and photon band structures. It is possible to have this band structure in certain synthesized materials. The Chern numbers may correspond to the number of edge states. One of the most interesting situation is $m = 1$. To exhibit $c_2^{(1)} = n + 1$, $c_2^{(2)} = -n$, the material may have $n + 1$ right chiral edge states and n left chiral edge states. In the context of photonic crystals, it may have $n+1$ uni-directional right-moving edge states, and n uni-directional left-moving edge states. These topological quantum numbers may manifest themselves in terms of the number of edge states, and may contribute to conductivities and transport properties of the materials.

In the situation that the fourth parameter ξ_4 can be integrated out, the expressions can be reduced to Chern-Simons integrals, because of the relation,

$$\epsilon_{dabc} \nabla_d [A^a_{ij} \nabla_b A^c_{ji} + i\frac{2}{3} A^a_{il} A^b_{lj} A^c_{ji}] = \frac{1}{4} \epsilon_{abcd} (\mathrm{tr} F^{ab} F^{cd}). \tag{11}$$

Therefore the reduced integration keeps the information of the four dimensional integral. In the case of momentum space (k_a, k_b, k_c) plus ξ_4, the integration after reducing on ξ_4 is over the Brillouin zone.

The four dimensional topological insulator can be characterized by Z invariant. In 4D it may be characterized by $c_2 \in \mathrm{Z}$. So here the system with $\mathrm{Z} \oplus \mathrm{Z}$ invariant may be mapped to doubled topological insulators in four spatial dimensions. Upon a reduction on the fourth parameter ξ_4, the system becomes a doubled three dimensional topological insulators. The three dimensional topological insulator have been characterized by Z_2 invariant.[7–9] The elements of Z_2 correspond to odd number or even number of Dirac points, which is related to the global property of the Brillouin zone.[7–9] The odd class are topological insulators, and the even class are normal insulators.

The fibration may be related to axion electrodynamics. An effective axion term can be induced in several ways[10,11] in three spatial dimensions and one time dimension. Similarly, in four spatial dimensions, there are effective Chern-Simons action that can be induced[10] in four spatial dimensions and one time dimension. The Chern-Simons term $A_\kappa \epsilon^{\kappa\mu\nu\lambda\rho}\partial_\mu A_\nu \partial_\lambda A_\rho$ is the one-loop effective term arising from integrating the fermion loop and the coefficient is given by the second Chern number in the momentum space of the fermion. Up on reduction on $\kappa = x_4$ direction, A_κ becomes $\hat{\theta}$ field.

In three spatial dimensions and one time dimension, the systems can effectively have axion term, or θ term, and have magneto-electric effects,

$$S = \frac{e^2}{16\pi h}(c_2^{(1)} + c_2^{(2)}) \int dt d^3x (\hat{\theta}\epsilon^{\mu\nu\lambda\rho}\partial_\mu A_\nu \partial_\lambda A_\rho), \tag{12}$$

$$\theta = (c_2^{(1)} + c_2^{(2)})\hat{\theta} = m\hat{\theta}, \tag{13}$$

where $A_\mu(x)$ is real space gauge field. When the system has time-reversal symmetry, the time-reversal symmetry and gauge symmetry require that $\theta = m\pi$, where m is an integer. This term is proportional to $\mathbf{E} \cdot \mathbf{B}$, and thus this will give magneto-electric polarization of the material.

If we consider the interface between two materials with different $\hat{\theta}$, in which case there is $\hat{\theta}_1$ for one material extending along $z < 0$, and $\hat{\theta}_2$ for the other material extending along $z > 0$. There is a jump $\hat{\theta}_1 - \hat{\theta}_2 = \Delta\hat{\theta}$ across the two sides of the interface. The time-reversal symmetry can be broken on this interface.[10,11] We can use the integration by parts $(\hat{\theta})\partial_z A_x \partial_t A_y = -A_x[(\partial_z \hat{\theta})\partial_t A_y]$ up to total derivatives. Since A_x is coupled to the current

j_x via $A_x j_x$, then at the interface we have that the induced current is

$$
\begin{aligned}
j_x &= \sigma_{xy} E_y, && (14)\\
j_x &= j_x^{(1)} + j_x^{(2)}, \qquad j_x^{(1)} = \sigma_{xy}^{(1)} E_y, \qquad j_x^{(2)} = \sigma_{xy}^{(2)} E_y. && (15)\\
j_x^{(1)} &= \frac{e^2}{h} \frac{(\hat{\theta}_1 - \hat{\theta}_2)}{2\pi} E_y c_2^{(1)} = (n+m) \frac{e^2}{h} \frac{(\hat{\theta}_1 - \hat{\theta}_2)}{2\pi} E_y, && (16)\\
j_x^{(2)} &= \frac{e^2}{h} \frac{(\hat{\theta}_1 - \hat{\theta}_2)}{2\pi} E_y c_2^{(2)} = -n \frac{e^2}{h} \frac{(\hat{\theta}_1 - \hat{\theta}_2)}{2\pi} E_y. && (17)
\end{aligned}
$$

The two conductivities have opposite signs. From the expression of the second Chern numbers, the conductance can be expressed as

$$
\begin{aligned}
\sigma_{xy}^{(1)} &= \frac{1}{4\pi^2} \int d^3k [\langle \psi^i | \partial_\mu \psi^j \rangle \langle \partial_\nu \psi^j | \partial_\lambda \psi^i \rangle + \frac{2}{3} \langle \psi^i | \partial_\mu \psi^j \rangle \langle \psi^j | \partial_\nu \psi^l \rangle \langle \psi^l | \partial_\lambda \psi^i \rangle] \frac{e^2}{h} \frac{(\hat{\theta}_1 - \hat{\theta}_2)}{2\pi} \epsilon^{\mu\nu\lambda},\\
\sigma_{xy}^{(2)} &= \frac{1}{4\pi^2} \int d^3k [\langle \psi^\alpha | \partial_\mu \psi^\beta \rangle \langle \partial_\nu \psi^\beta | \partial_\lambda \psi^\alpha \rangle + \frac{2}{3} \langle \psi^\alpha | \partial_\mu \psi^\beta \rangle \langle \psi^\beta | \partial_\nu \psi^\gamma \rangle \langle \psi^\gamma | \partial_\lambda \psi^\alpha \rangle] \frac{e^2}{h} \frac{(\hat{\theta}_1 - \hat{\theta}_2)}{2\pi} \epsilon^{\mu\nu\lambda},
\end{aligned}
\tag{18}
$$

where $\int d^3k = \int dk_x dk_y dk_z$, and where there is summation in the i, j, α, β labels of different occupied bands. The integration of the second Chern class over $I \times BZ$ reduces to the integration of two Chern-Simons forms on BZ.

The fibration is also related to band touching phenomena. There are nontrivial topological structures of occupied bands. There are also other unoccupied bands. We can diagonalize the Hamiltonian in the system, and it can take the form

$$
H(\mathbf{k}) = E_1(\mathbf{k}) \sum_{i=1,2} |i, \mathbf{k}\rangle \langle i, \mathbf{k}| + E_2(\mathbf{k}) \sum_{\alpha=1,2} |\alpha, \mathbf{k}\rangle \langle \alpha, \mathbf{k}| + \sum_{\gamma} E_\gamma(\mathbf{k}) |\gamma, \mathbf{k}\rangle \langle \gamma, \mathbf{k}| . \tag{19}
$$

We have that E_1, E_2 are energy eigenvalues of the two double bands. Those are occupied bands. We have written it in orthonormal basis. E_γ correspond to other unoccupied bands. The second Chern numbers of the occupied bands are $n+m, -n$ respectively. We propose that there may exist band structures with associated geometric phase that realize the exotic spheres.

When we tune the parameters in the model describing the material, the band structures can be deformed and changed. As long as there is no band touching that occurs during the tuning, the individual Chern number of each band remain unchanged, since it is topologically invariant. If when tuning the parameters, the band touching happens, then the Chern numbers of two bands that touch can change their individual Chern numbers. In these

situations, when tuning the parameters, the two bands first touch and then split. If we view the geometric phase gauge field as a fiber bundle over the parameter space, for example the three dimensional momentum space plus an additional parameter, then the transferring of Chern numbers during band-touching is a topology change of that fiber bundle. The base space is the parameter space, and the fiber is the geometric phase gauge field. The Chern number of the band may correspond to the number of edge states.

Consider the effective Hamiltonian of the two double bands,

$$H(\mathbf{k};\xi) = \left(\frac{E_1(\mathbf{k};\xi) + E_2(\mathbf{k};\xi)}{2}\right) \mathrm{I}_{4\times 4} - \left(\frac{E_1(\mathbf{k};\xi) - E_2(\mathbf{k};\xi)}{2}\right) \vec{\Gamma} \cdot \vec{\omega}(\mathbf{k};\xi), \tag{20}$$

where we write it in terms of 4×4 Hamiltonian $H(\mathbf{k};\xi)$, and where $\vec{\omega} \cdot \vec{\omega} = 1$, and Γ denotes Gamma matrices and ξ here denotes a parameter in the model Hamiltonian, for example spin-orbit coupling. If the band touching happens at a point near $(\hat{\mathbf{k}}; \hat{\xi})$, we draw a surface Σ_3 enclosing that point. The Chern number transfer between the two bands is therefore

$$\hat{n} = \frac{1}{8\pi^2} \int_{\Sigma_3} \langle \vec{\omega} \,| \vec{\omega} d\vec{\omega} \wedge d\vec{\omega} \wedge d\vec{\omega} \rangle \,. \tag{21}$$

This is the Chern number that is transferred between the two bands.

Starting from the state corresponding to $c_2^{(1)} = n + m,\ c_2^{(2)} = -n$, we can tune the parameters in the model, for example, the spin-orbit coupling, or strain, or magnetic field, so as to change the band structure to make the band touching point between the two bands happen. The two bands then split by tuning these parameters. When the bands touch and then split, they transfer Chern number $\Delta c_2 = \hat{n}$, and then the state becomes $c_2^{(1)} = n' + m,\ c_2^{(2)} = -n'$, in which $n' = n + \hat{n}$. From the point of view of instantons on the base space of the exotic sphere fibration, this transition between the two bands correspond to the transfer of $\hat{n}$ instantons between the two $su(2)$ gauge fields. This also corresponds to the topological change transition between exotic sphere fibrations with different n. The same procedure of band touching and Chern number transfer can be performed many times. This generates different fibrations with $c_2^{(1)} = n + m,\ c_2^{(2)} = -n$, and exotic spheres with $c_2^{(1)} = n + 1,\ c_2^{(2)} = -n$. The change of Chern numbers can be mapped to the topology change of the fiber bundle. These transitions may relate different n with fixed m.

Those states with fixed $m = 1$, fixed n belong to the same diffeomorphism class, and they may correspond to the situations that the topology of the band structure does not change, and in particular without band touching and Chern number transfer. Those with

fixed $m = 1$, but different n, are in the same homeomorphism class, but for different n (mod 28) are not in the same diffeomorphism class, and they may be non-adiabatically connected by band touchings.

Those with different m are not in the same homeomorphism class and may not be non-adiabatically connected. Since the two bands touch and split, the total Chern numbers of the two occupied bands, which is m, is topologically invariant and a conserved quantity of the total system. There are changes of the individual Chern numbers of each band, and there is a Chern number transfer between the two bands.

Many electron systems can be described by effective Hamiltonian that is quadratic in the Fermi field. In some situations there may contain terms that are quartic in the Fermi field. The quartic terms can give radiative loop corrections to the quadratic terms. In some situations that a mean field theory can be applied, and quartic term may be substituted by a quadratic term by a mean field approximation.

The system may be related to diverse systems, for example, topological insulators, quantum hall systems, models of Weyl semimetals, semiconductors, photonic crystals, and cold atom systems.

III. THEORETICAL DOUBLED TOPOLOGICAL INSULATOR MODEL

The 3D topological insulator materials include for example the Bi_2Te_3, Bi_2Se_3, Sb_2Te_3, and $Bi_{1-x}Sb_x$ (for example $Bi_{0.9}Sb_{0.1}$). The alloy $Bi_{0.9}Sb_{0.1}$ has five Fermi crossing points, and its theoretical model is more complicated than the situations of Bi_2Te_3, Bi_2Se_3, Sb_2Te_3, which have a single Dirac point. The topological insulator materials can be known by measuring whether there is odd or even number of Dirac points, which is related to the global property of the Brillouin zone.

The 3D Topological Insulator materials, for example[1–3] Bi_2Te_3, Bi_2Se_3, Sb_2Te_3, can be described by a simplified effective 4×4 model Hamiltonian, near the level-crossing point. They have large bulk gap of order $(1 \sim 3)\times 10^{-1}$ eV. The model with Se1-Bi1-Se2-Bi1′-Se1′ crystal structure have been studied in detail.[2] For example, for a Bi_2Se_3 crystal, in the effective model of the four band model, the basis of the state vector is

$$|P1^+_z, \uparrow\rangle,\ |P2^-_z, \uparrow\rangle,\ |P1^+_z, \downarrow\rangle,\ |P2^-_z, \downarrow\rangle \tag{22}$$

where $P1_z^+, P2_z^-$ are two p orbitals in the situations in a $\mathrm{Bi_2Se_3}$ crystal. Near the level-crossing point, the two bands touch each other. In this effective model, the four basis are from two orbitals and two spins. Let's abstract the state vector into

$$|+,\uparrow\rangle\,,\;\; |-,\uparrow\rangle\,,\;\; |+,\downarrow\rangle\,,\;\; |-,\downarrow\rangle\,. \tag{23}$$

We may introduce another $su(2)$ pseudospin space, in which we enlarge the 4×4 model Hamiltonian and 4 vector into 8×8 model Hamiltonian and 8 vector

$$|+,1,\uparrow\rangle\,,\;\; |-,1,\uparrow\rangle\,,\;\; |+,1,\downarrow\rangle\,,\;\; |-,1,\downarrow\rangle\,,\;\; |+,2,\uparrow\rangle\,,\;\; |-,2,\uparrow\rangle\,,\;\; |+,2,\downarrow\rangle\,,\;\; |-,2,\downarrow\rangle\,. \tag{24}$$

The pseudospin refers to the labels 1 and 2 in (24). There are potentially many different kinds of 3D topological insulator materials. It is in principle possible in the future to consider Interpenetrating Lattices of two topological insulator materials, or Interpenetrating Lattices of one topological insulator and one normal insulator material experimentally. Here, we only discuss it theoretically. The model Hamiltonian of the 8×8 model can be described as

$$H(\mathbf{k}) = \epsilon_0(\mathbf{k},\xi)\mathrm{I}_{8\times8} + \begin{bmatrix} g(\mathbf{k},\xi) & 0 \\ 0 & -g(\mathbf{k},\xi) \end{bmatrix} \otimes \mathrm{I}_{4\times4} + \begin{bmatrix} d^{(1)}(\mathbf{k},\xi)n_a^{(1)}(\mathbf{k},\xi) & 0 \\ 0 & d^{(2)}(\mathbf{k},\xi)n_a^{(2)}(\mathbf{k},\xi) \end{bmatrix} \otimes \Gamma_a. \tag{25}$$

$n_a^{(1)}(\mathbf{k},\xi)$ and $n_a^{(2)}(\mathbf{k},\xi)$ are unit-norm vectors mapped from $(\mathbf{k},\xi)$ space. It is a 8×8 model, doubled from 4×4 model.[10] The model is analogous to doubled topological insulators, and have two second Chern numbers

$$c_2^{(1)} = \frac{3}{8\pi^2}\int d^3k d\xi \epsilon^{abcde} n_a^{(1)}\partial_{k_1} n_b^{(1)}\partial_{k_2} n_c^{(1)}\partial_{k_3} n_d^{(1)}\partial_\xi n_e^{(1)} = m+n, \tag{26}$$

$$c_2^{(2)} = \frac{3}{8\pi^2}\int d^3k d\xi \epsilon^{abcde} n_a^{(2)}\partial_{k_1} n_b^{(2)}\partial_{k_2} n_c^{(2)}\partial_{k_3} n_d^{(2)}\partial_\xi n_e^{(2)} = -n. \tag{27}$$

These integral representations also give the second Chern numbers.

In that case, the boundary states may compose of $m+n$ right chiral fermion modes, and n left chiral fermion modes. The Hamiltonian density of these states in momentum space may be expressed as

$$H(\mathbf{k}) = \sum_{i=1,\ldots,m+n} \hbar v_i \psi_i^\dagger(\boldsymbol{\sigma}\cdot\mathbf{k})\psi_i + \sum_{j=1,\ldots,n} \hbar v_j \psi_j^\dagger(-\boldsymbol{\sigma}\cdot\mathbf{k})\psi_j. \tag{28}$$

In general this fibration (8, 9) may be mapped to $m+n$ right chiral modes, and n left chiral modes. The total helicity number is m.

It can be realized in Interpenetrating Lattices of two kinds of insulator materials. In the context of topological insulators in three spatial dimensions, the situation with the odd number of edge states is topologically robust. Since one can perform perturbations to the system and a pair of Dirac cones can be coupled and then gapped after re-diagonalization of the Hamiltonian. For the odd number of Dirac cones, such perturbations will always leave at least one Dirac cone un-gapped.

For $m = 2$, it can be realized in Interpenetrating Lattices of two kinds of topological insulator materials. For $m = 1$, it can be realized in Interpenetrating Lattices of one kind of topological insulator material, and one kind of normal insulator material.

Because of the $u(1)$ symmetry, the electric current in the system is exactly conserved current. Similar to the discussion in section II, the electric charge current is

$$j_x^{(1)} = \frac{e^2}{h}\frac{(\hat{\theta}_1^{(1)} - \hat{\theta}_2)}{2\pi}c_2^{(1)}E_y, \tag{29}$$

$$j_x^{(2)} = \frac{e^2}{h}\frac{(\hat{\theta}_1^{(2)} - \hat{\theta}_2)}{2\pi}c_2^{(2)}E_y, \tag{30}$$

at the interface between the Interpenetrating Lattices of the two materials with $\hat{\theta}_1^{(1)}$, $\hat{\theta}_1^{(2)}$ respectively, and another material with $\hat{\theta}_2$.

In the context of Interpenetrating Lattices, the enlargement from 4×4 to 8×8 is due to two types of interweaving lattice site $\mathrm{L}^{(1)}$, $\mathrm{L}^{(2)}$. Measurement associated with particular sublattice $\mathrm{L}^{(1)}$ or $\mathrm{L}^{(2)}$ selects the corresponding Chern number.

IV. PHOTONIC CRYSTALS

We may connect these fibrations to electron band and photon band. The photonic bands are parallel and similar to electronic bands. Photonic crystal with bulk band-gap, and gapless edge modes are in some aspects similar to topological insulator. It can have several bulk band-gaps. It may have special edge states. Since the material has bulk band-gap for the photon, it will forbid the bulk transmission of the photons in certain range of frequencies, for example $\omega_2 < \omega < \omega_1$. There can be surface band that are within the band-gap region of the bulk bands.

There are many ways to engineer photon bands in photonic crystals, and there are typically many closely-spaced bands. So there are many possibilities to have several Chern

numbers. There are Dirac points near band touching points. The photon bands also have geometric phases. The 2D photonic crystals can be made by periodic array of cylinders of dielectric medium, with lattice structure in x, y directions. The geometric phase of 2D photonic crystal can be defined and its first Chern number is given by integration of the field strength of the Berry phase gauge field in the 2D momentum space (k_x, k_y), for example.[12]

The 3D photonic crystals (PhC) and 2D photonic crystals (PhC) have a difference that the 2D photonic crystals have extra translational symmetry in z direction. The 3D photonic crystals can be made by 3D periodic arrays (or lattices) of dielectric spheres, or alternatively by 3D periodic arrays (lattices) of air holes in dielectric medium, or by 3D meshes of dielectric medium. There can be a limit that the lattice spacing along z direction is much smaller than the lattice spacings in x, y directions, and under such limit it cross over to 2D system. One can also define a conductivity of edge modes of photons in 3D.

The band topology can be realized also in three dimensional photonic crystals. The geometric phase can also be similarly expressed

$$\mathcal{A}^a_{ij}(\mathbf{k}) = \mathrm{Im}\left(\frac{\Big(\boldsymbol{u}_i(\mathbf{k}), \tilde{B}^{-1}(\omega_j(\mathbf{k}))\nabla_{k_a}\boldsymbol{u}_j(\mathbf{k})\Big)}{\sqrt{\Big(\boldsymbol{u}_i(\mathbf{k}), \tilde{B}^{-1}(\omega_i(\mathbf{k}))\boldsymbol{u}_i(\mathbf{k})\Big)\Big(\boldsymbol{u}_j(\mathbf{k}), \tilde{B}^{-1}(\omega_j(\mathbf{k}))\boldsymbol{u}_j(\mathbf{k})\Big)}}\right). \tag{31}$$

$$\mathcal{A}^a_{\alpha\beta}(\mathbf{k}) = \mathrm{Im}\left(\frac{\Big(\boldsymbol{u}_\alpha(\mathbf{k}), \tilde{B}^{-1}(\omega_\beta(\boldsymbol{k}))\nabla_{k_a}\boldsymbol{u}_\beta(\mathbf{k})\Big)}{\sqrt{\Big(\boldsymbol{u}_\alpha(\mathbf{k}), \tilde{B}^{-1}(\omega_\alpha(\mathbf{k}))\boldsymbol{u}_\alpha(\mathbf{k})\Big)\Big(\boldsymbol{u}_\beta(\mathbf{k}), \tilde{B}^{-1}(\omega_\beta(\mathbf{k}))\boldsymbol{u}_\beta(\mathbf{k})\Big)}}\right). \tag{32}$$

The round bracket denotes contraction of spatial components of the field variables.[12] Here we include non-abelian geometric phases. The i, j labels a double band and takes values 1 or 2. The α, β labels a different double band and takes values 1 or 2. We have assumed almost degeneracy $\omega_i \simeq \omega_j$, and $\omega_\alpha \simeq \omega_\beta$. We assume that there are two almost doubly degenerate bands in the band structure.

$B^{-1}(r,\omega)$ is an 6×6 block-diagonal permittivity-permeability tensor

$$B^{-1}(r,\omega) = \begin{bmatrix} \epsilon_{ab}(r,\omega) & 0 \\ 0 & \mu_{ab}(r,\omega) \end{bmatrix}. \tag{33}$$

$\tilde{B}^{-1}(\omega)$ has taken into account frequency dependence,[12]

$$\tilde{B}^{-1}(r,\omega) = B^{-1}(r,\omega) + \omega\partial_\omega B^{-1}(r,\omega). \tag{34}$$

The $\epsilon_{ab}(r,\omega)$, $\mu_{ab}(r,\omega)$ are 3×3 permittivity tensor and permeability tensor, and they generally have off-diagonal components. $\tilde{B}^{-1}(\omega(\mathbf{k}))$ is a nontrivial tensor due to the dielectric medium, and they have frequency dependence.[12]

The $\boldsymbol{u}_i(\mathbf{k},r)e^{i\mathbf{k}\cdot r}$ is the Bloch state of the 6-component complex vector $(\tilde{E}_i(\mathbf{k},r),\tilde{H}_i(\mathbf{k},r))$, of the electromagnetic fields of the normal mode with momentum vector $\mathbf{k}$ and frequency $\omega_i(\mathbf{k})$.

One can define a Chern-Simons integral,

$$I=\frac{1}{4\pi}\int dk_x dk_y dk_z \epsilon_{abc}[\mathcal{A}^a_{ij}\nabla_{k_b}\mathcal{A}^c_{ji}+i\frac{2}{3}\mathcal{A}^a_{il}\mathcal{A}^b_{lj}\mathcal{A}^c_{ji}]. \tag{35}$$

The integral is in the 3D momentum space (k_x,k_y,k_z) of the 3D photonic crystal, and summation of the scripts are assumed in the notations.

Because of the relation,

$$\epsilon_{dabc}\nabla_d[\mathcal{A}^a_{ij}\nabla_b\mathcal{A}^c_{ji}+i\frac{2}{3}\mathcal{A}^a_{il}\mathcal{A}^b_{lj}\mathcal{A}^c_{ji}]=\frac{1}{4}\epsilon_{abcd}(\mathrm{tr}F^{ab}F^{cd}) \tag{36}$$

the four dimensional integral of

$$\frac{1}{4}\int d\xi_a d\xi_b d\xi_c d\xi_d \ \epsilon_{abcd}(\mathrm{tr}F^{ab}F^{cd}) \tag{37}$$

can be reduced to three dimensional integral of

$$\int d\xi_a d\xi_b d\xi_c[\mathcal{A}^a_{ij}\nabla_b\mathcal{A}^c_{ji}+i\frac{2}{3}\mathcal{A}^a_{il}\mathcal{A}^b_{lj}\mathcal{A}^c_{ji}]. \tag{38}$$

Therefore the Chern-Simons integral has the information of the four dimensional integral that is associated with the c_2.

For particularly engineered 3D photonic crystals, there could be two second Chern numbers $c_2^{(1)}, c_2^{(2)}$, whose values may correspond to the numbers of right-moving and left-moving boundary states. This type of band structure can also be realized in Interpenetrating Lattices of two photonic crystal materials PhC and PhC$'$, experimentally. In the latter case, $c_2^{(1)}$, $c_2^{(2)}$ correspond to the two materials respectively. The Chern numbers may correspond to the number of boundary states, or uni-directional one-way propagating states on the boundary. This is independent of boson or fermion statistics. Photons can have right circular polarization and left circular polarization. In this context, the photon's left or right polarization pattern of the boundary photon states would be interesting physical observable.

There can be a limit that the lattice spacing along z direction is much smaller than the lattice spacings in x, y directions, and the 3D system can crossover to the 2D system. The crossover relation between 3D TI and 2D TI in some aspects may be similar to the relation between 3D PhC and 2D PhC.

V. HETEROSTRUCTURE OF TI/NI/TI/NI′

In this section we discuss heterostructures of periodic units of TI/NI/TI/NI′ materials. The periodic heterostructure of TI/NI has been devised.[13,14] The TI/NI stands for Topological Insulator/Normal Insulator. In periodic TI/NI model,[13,14] there are two kinds of interfaces, NI/TI and TI/NI. In the periodic TI/NI/TI/NI′ model, there are four kinds of surfaces, NI/TI, TI/NI′, NI′/TI, TI/NI. These materials are arranged along the z direction layer by layer, from top to bottom direction. Here we make the normal insulators NI and NI′ on the two sides of the same topological insulator to be different. The difference of NI and NI′ introduces another $su(2)$ space, the ρ-space. We make the parameters of two kinds of TI/NI, TI/NI′ junctions to be different, so in each periodic unit, there are four materials. There is experimental method to make the heights of two normal insulators to be the same, while making the tunnelings of the surface electrons across the two kinds of normal insulators to be different. This type of structure can be experimentally performed by many layers of periodic heterostructure of thin films.

In each periodic unit, there are TI, NI, TI, NI′ structures. There are surface electrons in upper surface and lower surface of the TI materials (in x, y directions). The model Hamiltonians are built from the states on the interfaces, from the surface states of TI's. Adding the normal insulator materials can perturb the surface Hamiltonian by adding tunneling terms. The periodic structure is along the z direction. The periodic structure then make the states become bulk states of the engineered structure.

The model Hamiltonian is

$$
\begin{aligned}
H \;=\; & \sum_{\boldsymbol{k}_\perp, i, j} [(\hbar v_F \tau^z (\hat{z} \times \boldsymbol{\sigma}) \cdot \mathbf{k}_\perp + \Delta_s \tau^x + b_z \sigma^z + b_x \sigma^x)(\delta_{i,2j} + \delta_{i,2j+1}) \\
& + \frac{1}{2}\tau^+ (\Delta_1 \delta_{i,2j+1} + \Delta_2 \delta_{i,2j}) + \frac{1}{2}\tau^- (\Delta_1 \delta_{i,2j} + \Delta_2 \delta_{i,2j+1}) \Big] c^\dagger_{\boldsymbol{k}_\perp i} (c_{\boldsymbol{k}_\perp 2j+1} + c_{\boldsymbol{k}_\perp 2j}). \quad (39)
\end{aligned}
$$

This is generalized from the model Hamiltonian of the TI/NI model with two structures in each periodic unit.[13] τ^x, τ^y, τ^z are Pauli matrices, which act on the pseudospin space of

upper and lower surfaces, and $\tau^+ = \tau^x + i\tau^y, \tau^- = \tau^x - i\tau^y$. The $\mathbf{k}_\perp$ is the momentum in x, y directions. The i and $2j, 2j+1$ label different topological insulator layers. The Hamiltonian (39) can describe the periodic structure of topological insulators stacked together with normal insulators NI and NI′ in between, separating the topological insulators. The $b_z\sigma^z + b_x\sigma^x$ term in (39) describes spin splitting of the surface states, that can be induced by doping each TI layer with magnetic impurities. Δ_s describes the tunneling between the two surfaces of the same topological insulator. Δ_1 and Δ_2 describe the tunneling between the surfaces of two nearby topological insulators through the material in the middle, which are the NI and NI′ respectively. The Δ_1 and Δ_2 parameters have different sizes, and can be the same under the limit $\Delta_2/\Delta_1 \to 1$. The spacing of the periodic structure is d, and the total number of the periodic units is N. The parameters for TI materials are surface Fermi velocity v_F, b_z, b_x and tunneling Δ_s. The parameters for NI materials are the tunnelings Δ_1, Δ_2. The $b_z\sigma^z + b_x\sigma^x$ is a time-reversal symmetry breaking term.

There are several differences between the configurations here and the configurations in previous discussion.[13,14] In the configurations there,[13,14] there are two structures, the topological insulator and normal insulator in each unit. Here, there are four structures in each periodic unit, the TI, NI, TI, NI′. Here, we turn on the magnetic term in both z and x directions.

Making a Fourier transformation along the z direction,

$$c^\dagger_{\boldsymbol{k}_\perp,l} = \frac{1}{\sqrt{N}} \sum_{k_z} c^\dagger_{\boldsymbol{k}} e^{-ik_z ld}, \tag{40}$$

where N is the total number of the periodic units, the 3D momentum-space Hamiltonian is a 8×8 Hamiltonian,

$$H = \sum_{\boldsymbol{k}} c^\dagger_{\boldsymbol{k}} H(\mathbf{k}) c_{\boldsymbol{k}}, \tag{41}$$

$$H(\mathbf{k}) = \begin{bmatrix} \varepsilon+b_z\sigma^z+b_x\sigma^x & \Delta_s \mathrm{I}_\sigma & 0 & \Delta_2 e^{ik_z d}\mathrm{I}_\sigma \\ \Delta_s \mathrm{I}_\sigma & -\varepsilon + b_z\sigma^z+b_x\sigma^x & \Delta_1 \mathrm{I}_\sigma & 0 \\ 0 & \Delta_1 \mathrm{I}_\sigma & \varepsilon+b_z\sigma^z+b_x\sigma^x & \Delta_s \mathrm{I}_\sigma \\ \Delta_2 e^{-ik_z d}\mathrm{I}_\sigma & 0 & \Delta_s \mathrm{I}_\sigma & -\varepsilon + b_z\sigma^z+b_x\sigma^x \end{bmatrix}, \tag{42}$$

where $\varepsilon = \hbar v_F(\hat{z}\times\boldsymbol{\sigma})\cdot\mathbf{k}$. The Hamiltonian here is 8×8. Because another $su(2)$ ρ-space is

introduced when $\Delta_2 \neq \Delta_1$, the Hamiltonian is enlarged from 4×4 to 8×8.

We introduce a $su(2)$ space, ρ-space, where ρ^x, ρ^y, ρ^z are Pauli matrices. The Hamiltonian can be expressed as

$$\begin{aligned} H(\mathbf{k}) &= [\hbar v_F \tau^z \otimes (\hat{z} \times \boldsymbol{\sigma}) \cdot \mathbf{k} + \Delta_s \tau^x \otimes \mathrm{I}_\sigma + \mathrm{I}_\tau \otimes (b_z \sigma^z + b_x \sigma^x)] \otimes \mathrm{I}_\rho \\ &\quad + \frac{1}{2}[\tau^+ \Delta_1 + \tau^- \Delta_2 e^{ik_z d}]\rho^+ \frac{1}{2} \otimes \mathrm{I}_\sigma + \frac{1}{2}[\tau^- \Delta_1 + \tau^+ \Delta_2 e^{-ik_z d}]\rho^- \frac{1}{2} \otimes \mathrm{I}_\sigma, \end{aligned} \tag{43}$$

where $\rho^+ = \rho^x + i\rho^y, \rho^- = \rho^x - i\rho^y,$ and I_ρ is the identity in ρ-space.

In the special case, when $b_x = 0,$ making the transformation $\tau^\pm \to \tau^\pm \sigma^z, \sigma^\pm \to \sigma^\pm \tau^z$, we find

$$H(\mathbf{k}) = [\hbar v_F (\hat{z} \times \boldsymbol{\sigma}) \cdot \mathbf{k} + b_z \sigma^z] \ \mathrm{I}_\tau \otimes \mathrm{I}_\rho + \sigma^z \Sigma, \tag{44}$$

$$\Sigma = [\Delta_s \tau^x \otimes \mathrm{I}_\rho + \frac{1}{2}\tau^+ (\Delta_1 \rho^+ + \Delta_2 e^{-ik_z d} \rho^-) \frac{1}{2} + \frac{1}{2}\tau^- (\Delta_1 \rho^- + \Delta_2 e^{ik_z d} \rho^+) \frac{1}{2}]. \tag{45}$$

Σ does not contain σ, but only τ, ρ operators, so it commutes with $[\hbar v_F (\hat{z} \times \boldsymbol{\sigma}) \cdot \mathbf{k} + b_z \sigma^z] \ \mathrm{I}_\tau \otimes \mathrm{I}_\rho$, and commutes with the Hamiltonian, we can replace it by its eigenvalues, $\Sigma_\pm$. We find

$$\begin{aligned} &\pm \Sigma_\pm = \\ &\pm \left(\frac{1}{2}(\Delta_1^2 + \Delta_2^2) + \Delta_s^2 \mp \sqrt{\frac{1}{4}(\Delta_1^2 - \Delta_2^2)^2 + (\Delta_1^2 + \Delta_2^2)\Delta_s^2 + 2\Delta_s^2 \Delta_1 \Delta_2 \cos(k_z d)} \right)^{\frac{1}{2}}, \end{aligned} \tag{46}$$

and

$$H_{\pm\pm} = \hbar v_F (\hat{z} \times \boldsymbol{\sigma}) \cdot \mathbf{k} + b_z \sigma^z \pm \Sigma_\pm \sigma^z. \tag{47}$$

The first $\pm$ and second $\pm$ subscripts in $H_{\pm\pm}$ in (47) denote the $\pm$ in front of $\Sigma_\pm$, and the subscript of $\Sigma_\pm$, respectively.

The energy eigenvalues are

$$E = \pm \sqrt{\hbar^2 v_F^2 \mathbf{k}_\perp^2 + (b_z \pm \Sigma_\pm)^2}, \tag{48}$$

where $\pm \Sigma_\pm$ is in (46).

The Weyl node happens at, for example, when $b_z - \Sigma_- = 0$. For simplicity, we now denote b_z as b. The locations are

$$k_z = \frac{2\pi}{d} \pm k_0, \tag{49}$$

$$k_0 = \frac{2}{d} \arccos(\mp \frac{1}{2\sqrt{\Delta_1 \Delta_2} \Delta_s} [b^4 - 2(\Delta_1^2 + \Delta_2^2 + 2\Delta_s^2) b^2 + 4(\Delta_1 \Delta_2 + \Delta_s^2)^2]^{\frac{1}{2}}). \tag{50}$$

This state is very similar to a wave-packet of electrons whose k_z centers around the particular value $\frac{2\pi}{d} \pm k_0$. In this situation, the Weyl nodes are centered around $(k_x, k_y, k_z) = (0, 0, \frac{2\pi}{d} \pm k_0)$. So this means that the material only allows the transmission of the state with prescribed range of momentum. The limit $\Delta_2/\Delta_1 \to 1$ reduces to previous discussion,[13,14] in which case both Δ_1, Δ_2 equal to Δ_d.

The expansion around the band touching point $b_z - \Sigma_- = 0$ gives

$$
\begin{aligned}
H_{--} &= \hbar v_F(\hat{z} \times \boldsymbol{\sigma}) \cdot \mathbf{k} \pm \hbar v_0 k_z \sigma^z && (51) \\
&= \hbar v_F(\sigma^x k_y - \sigma^y k_x) \pm \hbar v_0 \sigma^z k_z && (52)
\end{aligned}
$$

where we redefined $k_z - (\frac{2\pi}{d} - k_0) \to k_z$, and where

$$
\hbar v_0 = \frac{\Delta_s^2 \Delta_1 \Delta_2 \frac{d}{2b} \sin(k_0 d)}{\Delta_s^2 - b^2 + \frac{1}{2}(\Delta_1^2 + \Delta_2^2)}. \tag{53}
$$

Near the Weyl points, the dispersion is

$$
E(\mathbf{k}) = \pm\hbar\sqrt{v_F^2(k_x^2 + k_y^2) + v_0^2 k_z^2}. \tag{54}
$$

This is a Weyl fermion in three spatial dimensions, as described in (52). This Weyl fermion is half of the components of a Dirac fermion. These Weyl fermions come in pairs, around $k_z = \frac{2\pi}{d} \pm k_0$. The two Weyl fermions are separated in the $\mathbf{k}$ space and have opposite helicities. The heterostructure of topological insulators and normal insulators thus become Weyl semimetals.

If $\Delta_2/\Delta_1 \to 1$, the above reduces to

$$
\Sigma_\pm = \sqrt{\Delta_1^2 + \Delta_s^2 \mp 2\Delta_s \Delta_1 \cos(\frac{1}{2} k_z d)}, \tag{55}
$$

The branches with different signs can be understood as a phase shift in $\frac{1}{2}k_z d \to \frac{1}{2}k_z d + \pi$. The period when $\Delta_2 \neq \Delta_1$ is $\frac{2\pi}{d}$, and when $\Delta_2/\Delta_1 \to 1$ is enhanced to $\frac{4\pi}{d} = \frac{2\pi}{d/2}$. When taking the $\Delta_2/\Delta_1 \to 1$ limit, $\Delta_1 = \Delta_2 = \Delta_d$,

$$
\begin{aligned}
\Delta_1^2 + \Delta_s^2 - b^2 &= 2\Delta_s \Delta_1 \cos(\frac{1}{2} k_0 d), && (56) \\
\hbar v_0 &= \Delta_s \Delta_1 \frac{d}{2b} \sin(\frac{1}{2} k_0 d) && (57)
\end{aligned}
$$

which reduces to previous discussion[13,14] in the $\Delta_2/\Delta_1 \to 1$ limit.

When we tune the parameters b or the tunnelings, the band touching occurred and the transition[13] between insulators and Weyl semimetals is closely related to the topology change of the band structure on the parameter space.

There is another limit $\Delta_2/\Delta_1 \to 0$ limit, in which the tunneling across the NI′ material is taken to zero, so this is the limit when there is TI/NI/TI heterojunction.

The doping with magnetic impurities can be experimentally performed in, for example,[16] by for example Mn doped Bi_2Se_3. These heterostructures can be experimentally made by using topological insulator thin films, which have been demonstrated in experiments.[17]

These models of Weyl semimetals have bulk gapless modes at particular momentum vectors, near the above Weyl nodes, and these modes with the particular momentum vectors near the Weyl nodes conduct electric current as well as thermal current. These materials have electrical conductivity and thermal conductivity which can be measured and useful.

VI. HETEROSTRUCTURE OF TI/SC/TI/SC′

One can also replace the normal insulator materials discussed in the last section with superconductors (SC), and consider TI/SC/TI/SC′ heterostructures. One can also consider the model by changing the NI to superconductor (SC), and construct the model corresponding to TI/SC/TI/SC′ heterostructure. The superconductors can introduce couplings between opposite spins within the same surfaces (for both upper surface and lower surface), $|\Delta|e^{i\varphi}c^\dagger_{\boldsymbol{k}\uparrow}c^\dagger_{-\boldsymbol{k}\downarrow}$+h.c.. The parameters for SC and SC′ are slightly different.

Now the Hamiltonian is further enlarged by a κ-space. The $su(2)$ κ-space is due to particle-hole symmetry. The size or dimension of the state vector is doubled due to particle-hole symmetry. The periodic TI/SC model has been considered.[15] The surface Hamiltonian of each surface is further perturbed by a superconducting pairing term.

We again transform the Hamiltonian to momentum space via (40). We then make the transformation $\tau^\pm \to \tau^\pm\sigma^z, \sigma^\pm \to \sigma^\pm\tau^z$. The size of the Hamiltonian is 16×16. For TI/SC/TI/SC′ heterostructure, the model Hamiltonian in momentum space is

$$H = \sum_{\boldsymbol{k};\hat{\imath},\hat{\jmath}=\pm,\pm} c^\dagger_{\boldsymbol{k}\hat{\imath}} H_{\hat{\imath}\hat{\jmath}} c_{\boldsymbol{k}\hat{\jmath}} + \sum_{\boldsymbol{k};\hat{\imath}=\hat{\jmath}=\pm,\pm} (|\Delta|e^{i\varphi}c^\dagger_{\boldsymbol{k}\hat{\imath}\uparrow}c^\dagger_{-\boldsymbol{k}\hat{\jmath}\downarrow} + \text{h.c.}) \tag{58}$$

where the second term is superconducting pairing term with $\Delta = |\Delta|e^{i\varphi}$. $H_{\hat{\imath}\hat{\jmath}}$ is the Hamiltonian without adding the superconducting term, and $\hat{\imath}, \hat{\jmath}$ denote four blocks corresponding

to $\pm, \pm$ in (47).

These four eigenvalues of $H_{\hat{i}\hat{j}}$ correspond to sectors of $\tau^z, \rho^z = \pm 1, \pm 1$,

$$H_{\pm\pm} = \hbar v_F(\hat{z} \times \boldsymbol{\sigma}) \cdot \mathbf{k} + (b_z \pm \Sigma_\pm)\sigma^z \tag{59}$$

with the eigenvalues

$$\begin{aligned}&(b_z \pm \Sigma_\pm) \\ &= b \pm \left(\frac{1}{2}(\Delta_1^2 + \Delta_2^2) + \Delta_s^2 \mp \sqrt{\frac{1}{4}(\Delta_1 - \Delta_2)^2 + (\Delta_1^2 + \Delta_2^2)\Delta_s^2 + 2\Delta_s^2\Delta_1\Delta_2 \cos(k_z d)} \right)^{\frac{1}{2}}.\end{aligned} \tag{60}$$

When adding the superconducting term, the 4×4 Hamiltonians are

$$H^{\Delta}_{i=\pm\pm} = \frac{1}{2}\sum_{\boldsymbol{k}} \psi^\dagger_{k,i}(\hbar v_F(\hat{z} \times \boldsymbol{\sigma}) \cdot \mathbf{k}\ \mathrm{I}_\kappa + \sigma^z[(b_z \pm \Sigma_\pm)\mathrm{I}_\kappa + \frac{1}{2}(|\Delta|e^{i\varphi}\kappa^+ + |\Delta|e^{-i\varphi}\kappa^-)])\psi_{k,i} \tag{61}$$

where the basis is $\psi_{\boldsymbol{k},i} = (c_{\boldsymbol{k}i\uparrow}, c_{\boldsymbol{k}i\downarrow}, c^\dagger_{-\boldsymbol{k}i\downarrow}, c^\dagger_{-\boldsymbol{k}i\uparrow}),\ i = (\pm, \pm)$. The superscript Δ in $H^{\Delta}_{i=\pm\pm}$ denotes including the superconducting term. The first $\pm$ and second $\pm$ subscripts in $H^{\Delta}_{i=\pm\pm}$ in (61) denote $\tau^z, \rho^z = \pm 1, \pm 1$. There are four blocks corresponding to $(\pm, \pm)$. The $b_z\sigma^z$ term is a deformation of the quadratic term, and is due to the doping of magnetic impurities in the TI. $\kappa^x, \kappa^y, \kappa^z$ are Pauli matrices, and $\kappa^+ = \kappa^x + i\kappa^y$, $\kappa^- = \kappa^x - i\kappa^y$. The superconducting term was from a quartic term, and after a mean field treatment it becomes a quadratic term in the Hamiltonian.

For example, for $\tau^z, \rho^z = -1, -1$,

$$H^{\Delta}_{--} = \frac{1}{2}\sum_{\boldsymbol{k}} \psi^\dagger_{\boldsymbol{k},--}(\hbar v_F(\hat{z} \times \boldsymbol{\sigma}) \cdot \mathbf{k}\ \mathrm{I}_\kappa + \sigma^z[(b_z - \Sigma_-)\mathrm{I}_\kappa + \frac{1}{2}(|\Delta|e^{i\varphi}\kappa^+ + |\Delta|e^{-i\varphi}\kappa^-)])\psi_{\boldsymbol{k},--}. \tag{62}$$

In the matrix form in κ-space,

$$H^{\Delta}_{i=\pm\pm}(\mathbf{k}) = \begin{bmatrix} [\hbar v_F(\hat{z} \times \boldsymbol{\sigma}) \cdot \mathbf{k} + (b_z \pm \Sigma_\pm)\sigma^z] & |\Delta|e^{i\varphi}\sigma^z \\ |\Delta|e^{-i\varphi}\sigma^z & [\hbar v_F(\hat{z} \times \boldsymbol{\sigma}) \cdot \mathbf{k} + (b_z \pm \Sigma_\pm)\sigma^z] \end{bmatrix}. \tag{63}$$

The Hamiltonian in (63) can be diagonalized in κ-space. When it is diagonalized in κ-space, this is given by a transformation

$$H = \frac{1}{2}\sum_{\boldsymbol{k};i,j=(\pm,\pm)} \tilde{\psi}^\dagger_{i,\boldsymbol{k}} H^{\Delta}_{ij} \tilde{\psi}_{j,\boldsymbol{k}}, \tag{64}$$

with the basis of state vector

$$(\tilde{\psi}_{+,\boldsymbol{k}}, \tilde{\psi}^\dagger_{+,(-\boldsymbol{k})}, \tilde{\psi}_{-,\boldsymbol{k}}, \tilde{\psi}^\dagger_{-,(-\boldsymbol{k})}),$$

where[15]

$$\tilde{\psi}_{+,\boldsymbol{k}} = \frac{1}{\sqrt{2}} e^{-\frac{1}{2}i\varphi} c_{\boldsymbol{k}i\uparrow} + \frac{1}{\sqrt{2}} e^{\frac{1}{2}i\varphi} c^\dagger_{-\boldsymbol{k}i\downarrow}, \tag{65}$$

$$\tilde{\psi}_{-,\boldsymbol{k}} = -\frac{i}{\sqrt{2}} e^{-\frac{1}{2}i\varphi} c_{\boldsymbol{k}i\uparrow} + \frac{i}{\sqrt{2}} e^{\frac{1}{2}i\varphi} c^\dagger_{-\boldsymbol{k}i\downarrow}, \tag{66}$$

It can again be diagonalized in κ-space. For $\tau^z, \rho^z = -1, -1$, for $\kappa^z = \pm 1$,

$$H^{\Delta\pm}_{--} = \hbar v_F (\hat{z} \times \boldsymbol{\sigma}) \cdot \mathbf{k} + \sigma^z (b_z - \Sigma_- \pm |\Delta|), \tag{67}$$

where the superscript $\pm$ in $H^{\Delta\pm}_{--}$ denotes $\kappa^z = \pm 1$, and $\pm|\Delta|$ in (67) correspond to $\kappa^z = \pm 1$.

Similarly for the four sectors $\tau^z, \rho^z = \pm 1, \pm 1$,

$$H^{\Delta\pm}_{\pm\pm} = \hbar v_F (\hat{z} \times \boldsymbol{\sigma}) \cdot \mathbf{k} + \sigma^z (b_z \pm \Sigma_\pm \pm |\Delta|). \tag{68}$$

$|\Delta|$ effectively shifts $b_z \pm \Xi_\pm$. The eigenvalue is

$$E(\mathbf{k}) = \pm \sqrt{\hbar^2 v_F^2 \mathbf{k}_\perp^2 + (b_z \pm \Sigma_\pm \pm |\Delta|)^2}. \tag{69}$$

where $b_z \pm \Sigma_\pm$ are in (60).

The Bogoliubov-Weyl nodes near the band touching points are located at for example $b_z - \Sigma_\pm \pm |\Delta| = 0$. For $b_z - \Sigma_- \pm |\Delta| = 0$, they are

$$k_z = \frac{2\pi}{d} \pm k_0^\Delta, \tag{70}$$

$$k_0^\Delta = \frac{2}{d} \arccos(\mp \frac{1}{2\sqrt{\Delta_1 \Delta_2}\Delta_s} [(b \pm |\Delta|)^4 - 2(\Delta_1^2 + \Delta_2^2 + 2\Delta_s^2)(b \pm |\Delta|)^2 + 4(\Delta_1 \Delta_2 + \Delta_s^2)^2]^{\frac{1}{2}}) \tag{71}$$

and the Fermi velocity is

$$\hbar v_0 = \frac{\Delta_s^2 \Delta_1 \Delta_2 \frac{d}{2b} \sin(k_0 d)}{\Delta_s^2 - (b \pm |\Delta|)^2 + \frac{1}{2}(\Delta_1^2 + \Delta_2^2)}. \tag{72}$$

We have thus found the energy eigenvalues, the locations of Weyl nodes, and the Fermi velocity near the node.

Interestingly, Weyl superconducting phases can also be realized by triplet pairing phases.[18,19]

VII. OTHER RELEVANT MATERIALS AND DISCUSSION

The $su(2)$ geometric phase with two Chern numbers may occur also in other condensed matter systems or atomic and molecular systems. There are related discussions in other possible situations.[20–22] The Semiconductor model includes at least light hole (LH) and heavy hole (HH) bands. If both LH and HH are doubly degenerate, they can also exhibit $su(2)$ geometric phases with two Chern numbers, in the d-space. There are related discussions[20,21] to these aspects. It is possible to exhibit general value of Chern numbers, by for example multilayer heterostructures of particular semiconductors.

The cold atomic system with cold atom of a larger total angular momentum of $F = 3/2$, can also exhibit $su(2)$ geometric phase in the parameter space of paring condensates, for example.[22] It may also be relevant to Interpenetrating Lattices of two optical lattices of cold atom systems.

It may be interesting to see whether these fibrations can be realized concretely in these experimental settings.

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